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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS 3	OCT 07	EPFULL enhanced with full implementation of EPC2000
NEWS 4	OCT 07	Multiple databases enhanced for more flexible patent number searching
NEWS 5	OCT 22	Current-awareness alert (SDI) setup and editing enhanced
NEWS 6	OCT 22	WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS 7	OCT 24	CHEMLIST enhanced with intermediate list of pre-registered REACH substances
NEWS 8	NOV 21	CAS patent coverage to include exemplified prophetic substances identified in English-, French-, German-, and Japanese-language basic patents from 2004-present
NEWS 9	NOV 26	MARPAT enhanced with FSORT command
NEWS 10	NOV 26	MEDLINE year-end processing temporarily halts availability of new fully-indexed citations
NEWS 11	NOV 26	CHEMSAFE now available on STN Easy
NEWS 12	NOV 26	Two new SET commands increase convenience of STN searching
NEWS 13	DEC 01	ChemPort single article sales feature unavailable
NEWS 14	DEC 12	GBFULL now offers single source for full-text coverage of complete UK patent families
NEWS 15	DEC 17	Fifty-one pharmaceutical ingredients added to PS

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:11:05 ON 18 DEC 2008

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=> file registry
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.42       0.42

FILE 'REGISTRY' ENTERED AT 14:12:01 ON 18 DEC 2008
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STRUCTURE FILE UPDATES:   17 DEC 2008  HIGHEST RN 1086212-50-1
DICTIONARY FILE UPDATES:  17 DEC 2008  HIGHEST RN 1086212-50-1

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
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on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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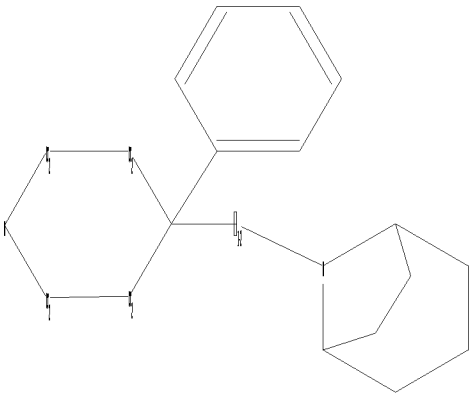

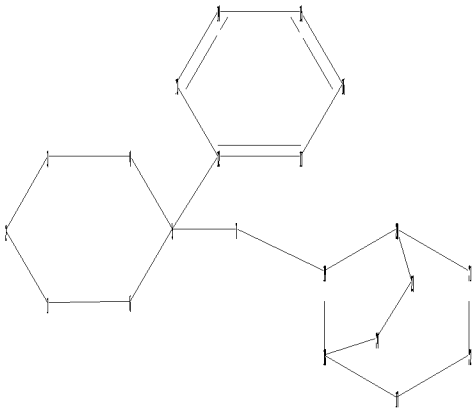

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7
ring nodes :
1  2  3  4  5  6  11  12  13  14  15  16  17  18  19  20  21  22  23  24
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5-7  5-12  7-19
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  11-12  11-16  12-13  13-14  14-15  15-16  17-18  17-22
18-19  18-24  19-20  20-21  20-23  21-22  23-24
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-19  17-18  17-22  18-19  18-24  19-20  20-21  20-23
21-22  23-24
exact bonds :
```

5-7 5-12
normalized bonds :
11-12 11-16 12-13 13-14 14-15 15-16

G1:Cb,Cy,Hy,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 11:Atom 12:Atom 13:Atom
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom

L1   STRUCTURE UPLOADED

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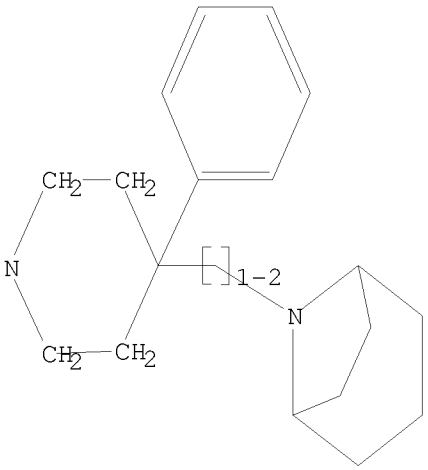
L1 HAS NO ANSWERS
L1   STR



G1 Cb,Cy,Hy,Ak

Structure attributes must be viewed using STN Express query preparation.

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FULL SEARCH INITIATED 14:13:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1834 TO ITERATE

100.0% PROCESSED   1834 ITERATIONS   1261 ANSWERS
SEARCH TIME: 00.00.01

L2   1261 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                       ENTRY   SESSION
FULL ESTIMATED COST   182.96   183.38

FILE 'CAPLUS' ENTERED AT 14:18:38 ON 18 DEC 2008

FILE COVERS 1907 - 18 Dec 2008 VOL 149 ISS 25
FILE LAST UPDATED: 17 Dec 2008 (20081217/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s l2
L3 2 L2

=> d l2 1-2 abs ibib hitstr
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

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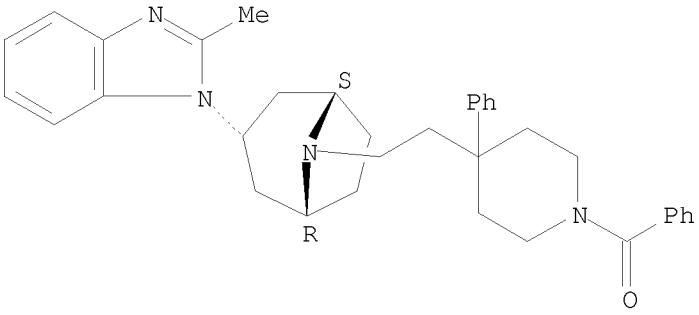
L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
AB We describe robust chemical approaches toward putative CCR5 scaffolds designed in our labs. Evaluation of analogs in the 125I-[MIP-1β] binding and Ba-L-HOS antiviral assays resulted in the discovery of 64 and 68 in the 4,4-disubstituted piperidine class H, both potent CCR5 ligands (pIC50 = 8.30 and 9.00, resp.) and HIV-1 inhibitors (pIC50 = 7.80 and 7.84, resp., in Ba-L-HOS assay). In addition, 64 and 68 were bioavailable in rodents, establishing them as lead mols. for further optimization toward CCR5 clin. candidates.
ACCESSION NUMBER: 2008:1154437 CAPLUS <<LOGINID::20081218>>
DOCUMENT NUMBER: 149:486141
TITLE: Discovery of Bioavailable 4,4-Disubstituted Piperidines as Potent Ligands of the Chemokine Receptor 5 and Inhibitors of the Human Immunodeficiency Virus-1
AUTHOR(S): Kazmierski, Wieslaw M.; Aquino, Christopher; Chauder, Brian A.; Deanda, Felix; Ferris, Robert; Jones-Hertzog, Deborah K.; Kenakin, Terrence; Koble, Cecilia S.; Watson, Christian; Wheelan, Pat; Yang, Hanbiao; Youngman, Michael
CORPORATE SOURCE: Infectious Diseases Center for Excellence in Drug Discovery, Molecular Discovery Research, Computational and Structural Chemistry, Drug Discovery, IT ID DMPK, Metabolic Pathways Center for Excellence in Drug Discovery, GlaxoSmithKline, Research Triangle Park, NC, 27709, USA

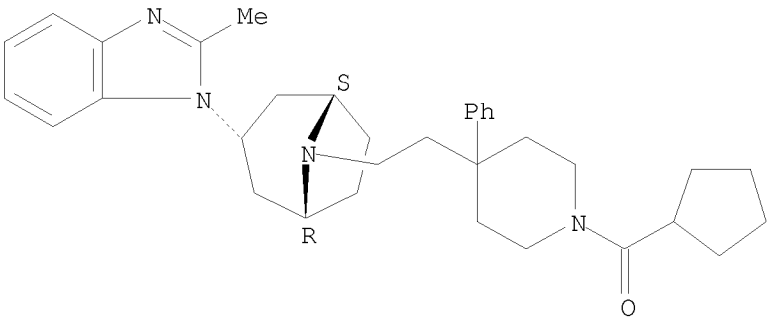
SOURCE: Journal of Medicinal Chemistry (2008), 51(20), 6538-6546
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 716344-87-5P 716344-88-6P 717101-60-5P
717101-63-8P 1071993-49-1P 1071993-56-0P
1072196-30-5P 1072196-31-6P 1072196-32-7P
1072196-33-8P 1072196-34-9P
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bioavailable piperidines as CCR5 ligands and HIV-1 inhibitors)
RN 716344-87-5 CAPLUS
CN Methanone, [4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenyl-1-piperidinyl]phenyl- (CA INDEX NAME)

Relative stereochemistry.



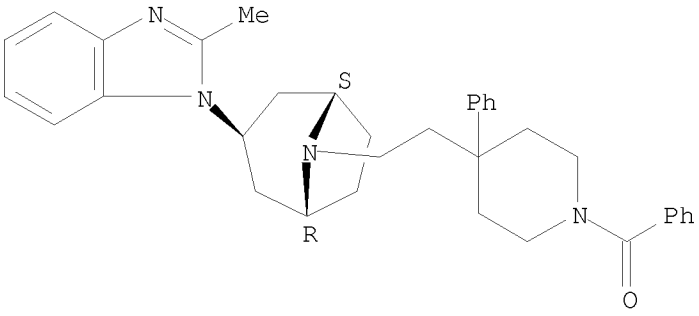
RN 716344-88-6 CAPLUS
CN Methanone, cyclopentyl[4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenyl-1-piperidinyl]- (CA INDEX NAME)

Relative stereochemistry.



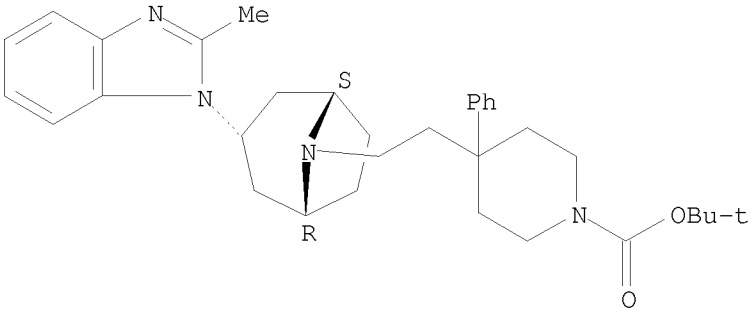
RN 717101-60-5 CAPLUS
CN Methanone, [4-[2-[(3-exo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenyl-1-piperidinyl]phenyl- (CA INDEX NAME)

Relative stereochemistry.

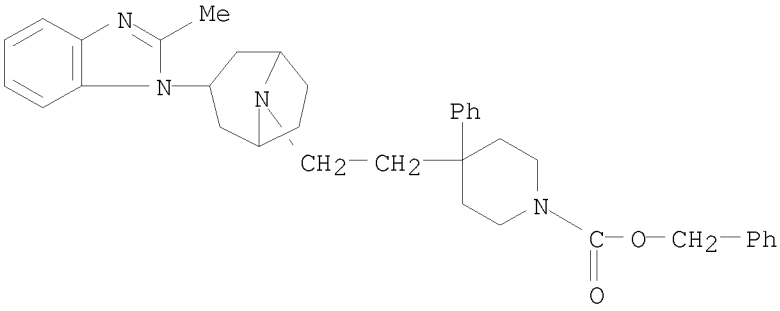


RN 717101-63-8 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

Relative stereochemistry.

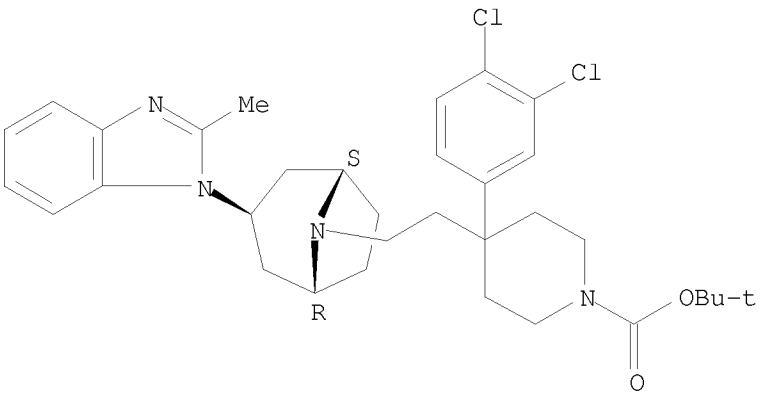


RN 1071993-49-1 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



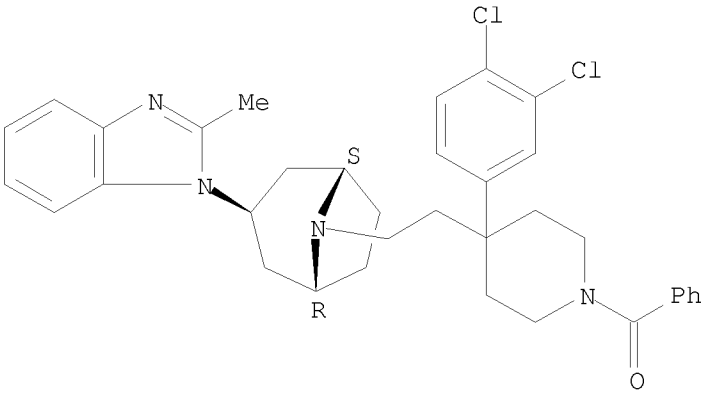
RN 1071993-56-0 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



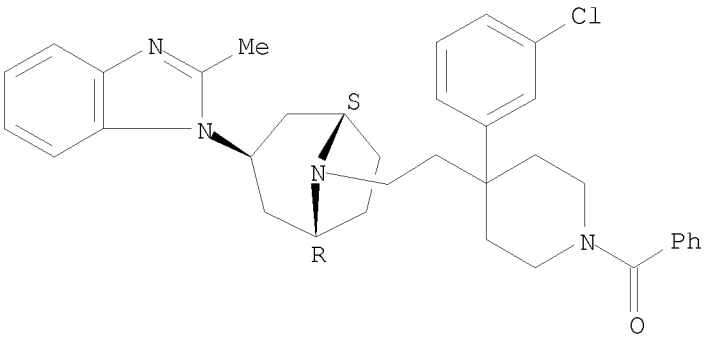
RN 1072196-30-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



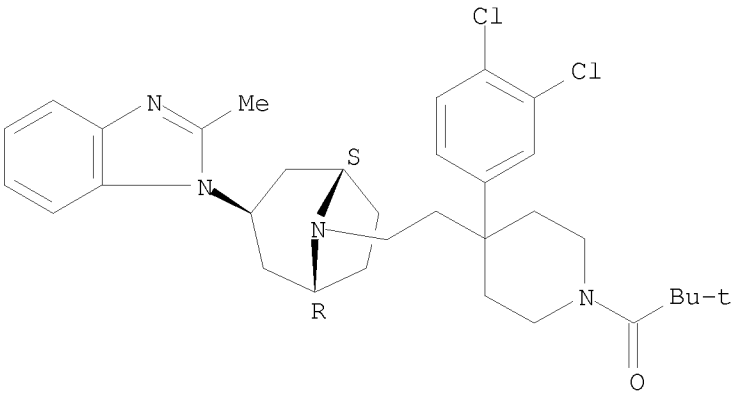
RN 1072196-31-6 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



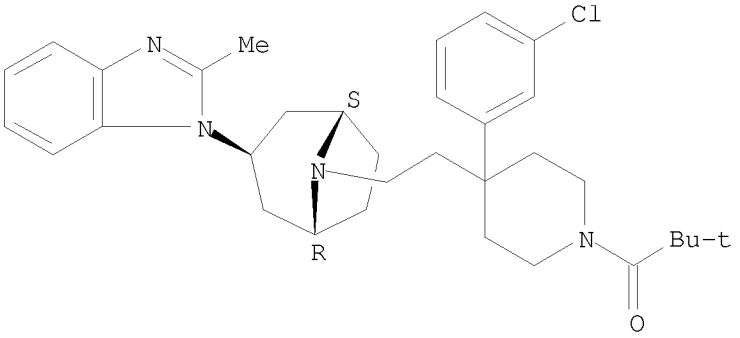
RN 1072196-32-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



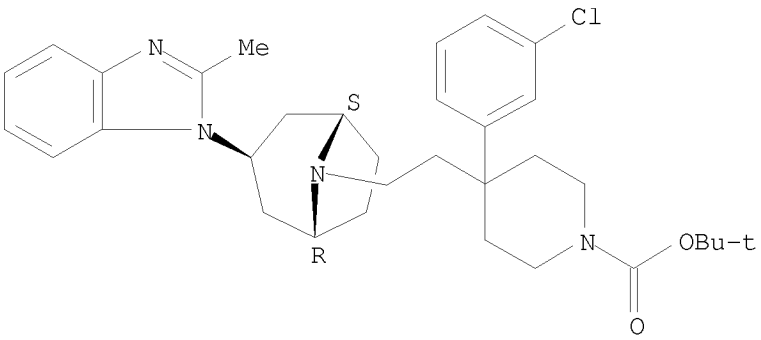
RN 1072196-33-8 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



RN 1072196-34-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



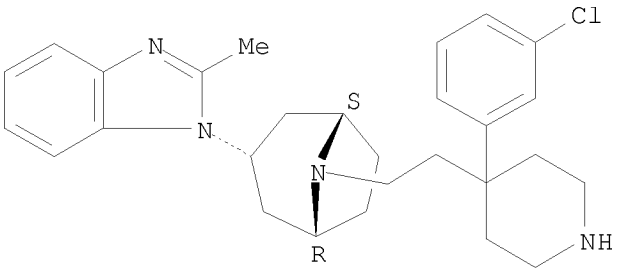
IT 716358-41-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bioavailable piperidines as CCR5 ligands and HIV-1 inhibitors)

RN 716358-41-7 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 8-[2-[4-(3-chlorophenyl)-4-piperidinyl]ethyl]-3-(2-methyl-1H-benzimidazol-1-yl)-, hydrochloride (1:2), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.



●2 HCl

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I [R1 = (optionally substituted) alkyl, aryl, heteroaryl, carbocyclyl; R2 = H, (optionally substituted) alkyl, aryl, heteroaryl, cycloalkyl, heterocycloalkyl, aralkyl, heteroarylalkyl, heteroarylcycloalkyl, aralkylcarbonyl, heteroarylsulfinyl; R3 = H, halo, cyano, trifluoromethyl, (optionally substituted) amino, acylamino, alkyl; X = C1-5 alkylene, optionally substituted with oxo or thioxo groups or halogen atoms, and optionally containing 1-3 oxygen, nitrogen, sulfur, or phosphorus atoms; Y = carbonyl, thiocarbonyl, 1,2-dioxoethylene, oxyalkylcarbonyl, sulfinyl, sulfonyl, oxycyanoimino, (optionally substituted) aminocarbonyl, carbonylamino, aminothiocarbonyl, oxyiminomethyl, thioiminomethyl, amino(cyanoimino)methyl, (cyanoimino)methyl, amino(acylimino)methyl, amino(sulfonylimino)methyl, amino(sulfinylimino)methyl, amino(alkoxyimino)methyl, amino(imino)methyl, (cyanoimino)methoxy, iminomethoxy, (cyanoimino)methanethiyl, alkylcarbonyloxy; A = saturated, partially saturated, or aromatic monocyclic ring with 5-6 atoms or a bicyclic ring with 8-10 members containing 0-5 nitrogen, oxygen, and/or sulfur atoms] such as II are prepared I are prepared as Ccr5 antagonists for the treatment of viral infections, (particularly HIV infection), related syndromes such as AIDS-related complex (ARC), progressive generalized lymphadenopathy, Kaposi's sarcoma, and neurol. conditions, and other diseases such as multiple sclerosis, rheumatoid arthritis, Crohn's disease, and immune-mediated disorders. The invention

compds. have pIC50 values of ≥5 in assays for Ccr5 antagonism. Piperidineacetaldehyde III is prepared in four steps from 4-phenyl-4-piperidinecarbonitrile by protection of the piperidine with Boc anhydride, reduction of the nitrile with diisobutylaluminum hydride, Wittig olefination with methoxymethylphosphonium chloride, and hydrolysis of the enol ether with catalytic p-toluenesulfonic acid monohydrate. The hydrochloride of endo-(benzimidazolyl)azabicyclooctane IV is prepared in five steps from tert-Bu endo-3-oxo-8-azabicyclo[3.2.1]octane-8-carboxylate; reductive amination with benzylamine, reductive cleavage of the benzyl group by palladium-mediated hydrogenation, a nucleophilic aryl substitution reaction with 1-fluoro-2-nitrobenzene, reduction of the nitro group by hydrogenation over palladium on carbon, and treatment with tri-Et orthoacetate followed by treatment with hydrochloric acid in ethanol. Coupling of III and IV by reductive amination with sodium triacetoxyborohydride, cleavage of the Boc group with hydrochloric acid in dioxane, and acylation with pivaloyl chloride and triethylamine yields II.

ACCESSION NUMBER: 2004:534173 CAPLUS <<LOGINID::20081218>>
DOCUMENT NUMBER: 141:89016
TITLE: Preparation of benzimidazolylazabicyclooctylethylpiperidines as Ccr5 antagonists for the treatment of HIV infection
INVENTOR(S): Kazmierski, Wieslaw Mieczyslaw; Aquino, Christopher Joseph; Bifulco, Neil; Boros, Eric Eugene; Chauder, Brian Andrew; Chong, Pek Yoke; Duan, Maosheng; Deanda, Felix, Jr.; Koble, Cecilia Suarez; Mclean, Ed Williams; Peckham, Jennifer Poole; Perkins, Angilique C.; Thompson, James Benjamin; Vanderwall, Dana
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA; et al.; et al.
SOURCE: PCT Int. Appl., 859 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004054974	A2	20040701	WO 2003-US39644	20031212
WO 2004054974	A3	20040902		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2509711	A1	20040701	CA 2003-2509711	20031212
AU 2003300902	A1	20040709	AU 2003-300902	20031212
EP 1569646	A2	20050907	EP 2003-813419	20031212
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BR 2003017230	A	20051025	BR 2003-17230	20031212
CN 1744899	A	20060308	CN 2003-80109628	20031212
JP 2006511554	T	20060406	JP 2004-560838	20031212
NO 2005002739	A	20050819	NO 2005-2739	20050607
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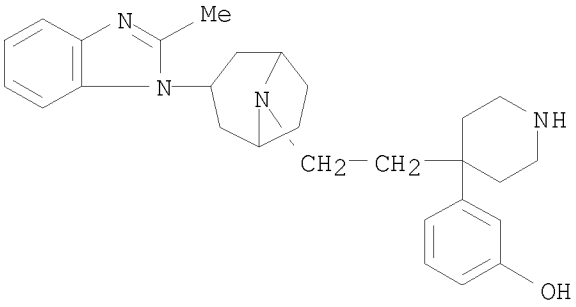
MX 2005PA06354	A	20050826	MX 2005-PA6354	20050613
IN 2005KN01328	A	20060630	IN 2005-KN1328	20050711

ZA 2005005600 A 20060927 ZA 2005-5600 20050712
PRIORITY APPLN. INFO.: US 2002-433634P P 20021213
WO 2003-US39644 W 20031212

OTHER SOURCE(S): MARPAT 141:89016

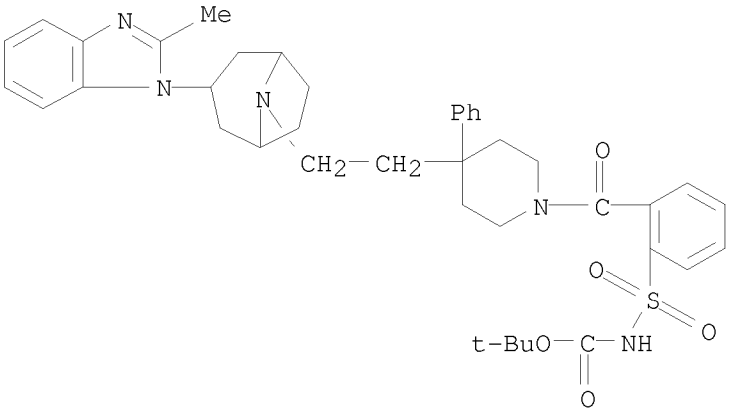
IT 1055923-67-5 1055923-68-6 1055923-71-1
1055923-72-2 1055923-73-3
RL: PRPH (Prophetic)
(Preparation of benzimidazolylazabicyclooctylethylpiperidines as Ccr5 antagonists for the treatment of HIV infection)

RN 1055923-67-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



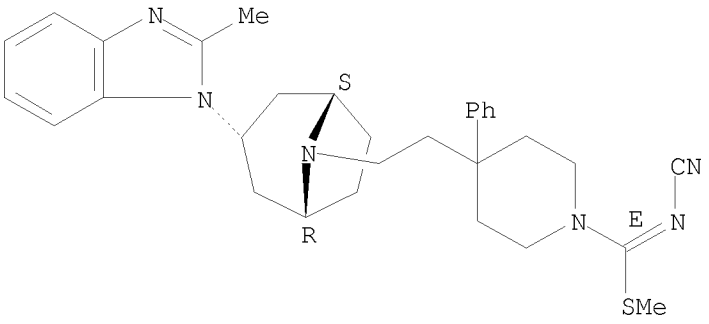
● HBr

RN 1055923-68-6 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



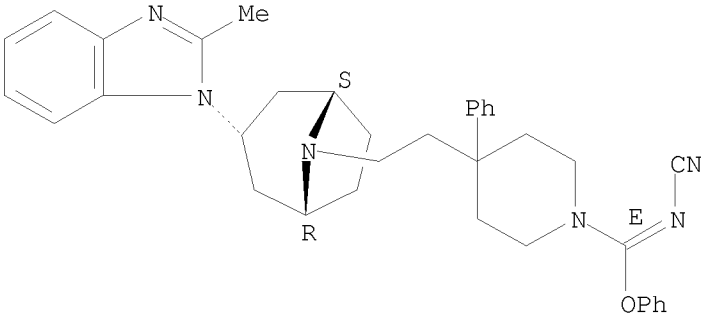
RN 1055923-71-1 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.
Double bond geometry as shown.

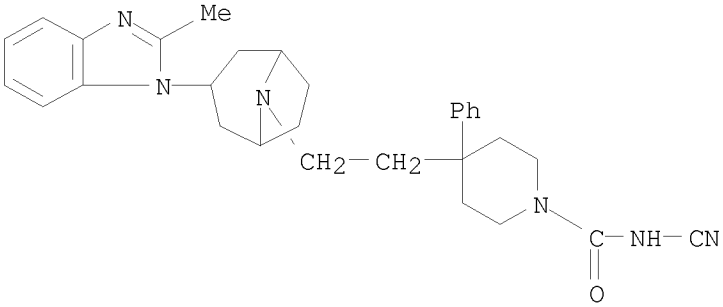


RN 1055923-72-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.
Double bond geometry as shown.



RN 1055923-73-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



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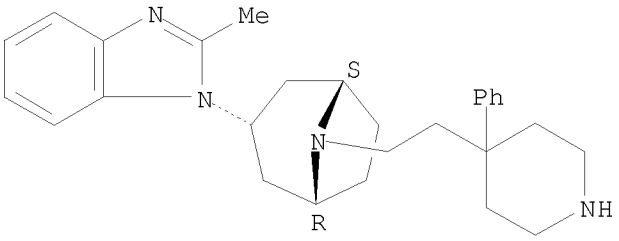
716355-15-6P 716355-18-9P 716355-24-7P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of benzimidazolylazabicyclooctylethylpiperidine Ccr5 antagonists in treatment of bacterial and viral infections and other diseases)

RN 716344-72-8 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 3-(2-methyl-1H-benzimidazol-1-yl)-8-[2-(4-phenyl-4-piperidinyl)ethyl]-, hydrochloride (1:2), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.



●2 HCl